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ABSTRACT

This resource document lists 36 books, papers, and reports dealing with various uses of computers in chemistry instruction; and describes several computer program packages available for use in teaching undergraduate, experimental laboratory, physical, and nuclear and X-ray chemistry, including biochemistry. Each program package is presented by reference number, name, description, subject, comment, language, and contact source for obtaining the package. (CHV)

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COMPUTERS IN CHEMISTRY TEACHING:
A BIBLIOGRAPHY AND INDEX OF CAL PACKAGES

N.J. Rushby
July 1979

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London SW7 2BX

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Bibliography ref no: 365

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Bibliography ref no: 525

DUBOIS, J E, LAURENT, D INFORMATICS AND NEW CONCEPTS IN CHEMISTRY IN COMPUTERS AND EDUCATION, LECARME, O AND LEWIS, R, EDS, IFIP NORTH HOLLAND, 1975, PP 437-442.

Bibliography ref no: 753

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Bibliography ref no: 754

JOHNSON, K J USE OF THE PITTSBURGH TIME-SHARING SYSTEM IN COMPUTER-ORIENTED CURRICULUM DEVELOPMENT IN CHEMISTRY PROC CONFERENCE ON COMPUTERS IN THE UNDERGRADUATE CURRICULA IOWA, JUNE 1970, PP 7,85-7,86.

Bibliography ref no: 770

JOHNSON, K J COMPUTERS AND CHEMICAL EDUCATION AT PITT PROC 2ND CONFERENCE ON COMPUTERS IN THE UNDERGRADUATE CURRICULA DARTMOUTH, JUNE 1971, PP 130-133.

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Bibliography ref no: 1147

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Bibliography ref no: 1385

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Bibliography ref no: 1483

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THE UNIVERSITY OF LANCASTER PAPER GIVEN AT THE CONFERENCE ON COMPUTERS
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DEAL, R.M. EXPLORING SIMPLE CHEMISTRY THEORY AT A CRT ACM INTERFACE,
V.5, NO.3, 1971. PP 119-124

Package ref no: 103

name: PREDPR ESP39
descrtn: RANDOM INFLUENCES ON POPULATION
subject: ENVIRONMENTAL CHEMISTRY AND CHEMICAL ENGINEERING DEGREE
LEVEL
lang: BASIC
contact: J.J.MATHEWS, DEPT OF APPLIED SCIENCE, THE QUEEN'S DRIVE,
EXETER, EX4 4QJ TEL 0392 77911

Package ref no: 104

name: REACT ESP54
descrtn: SIMULATION OF AN EXTERNALLY COOLED TUBULAR FLOW REACTOR WITH
GAS PHASE EXOTHERMIC REACTION
subject: ENVIRONMENTAL CHEMISTRY AND CHEMICAL ENGINEERING DEGREE
LEVEL
lang: BASIC
contact: J.J.MATHEWS, DEPT OF APPLIED SCIENCE, THE QUEEN'S DRIVE,
EXETER, EX4 4QJ TEL 0392 77911

Package ref no: 109

name: A501:PARTS 1, 2 AND 3
descrtn: DISSOCIATION CONSTANT OF N2O4
subject: FIRST YEAR LABORATORY EXPERIMENT:DEGREE
comment: CALCHEM
lang: PARTS 1 AND 2 IN STAF (VERSION OF LEEDS AUTHOR LANGUAGE)
PART 3 IS AVAILABLE IN BASIC OR CALC
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 110

name: A502
descrtn: FENC52+ EQUILIBRIUM
subject: FIRST YEAR DEGREE EXPERIMENTAL LABORATORY
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 111

name: A510
descrtn: PK OF AN INDICATOR
subject: FIRST YEAR DEGREE EXPERIMENTAL LABORATORY
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 112

name: A511
descrtn: DETERMINATION OF THE HYDROLYSIS CONSTANT OF ANALINE
HYDROCHLORIDE

subject: FIRST YEAR DEGREE LEVEL EXPERIMENTAL LABORATORY
comment: CALCHEM
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 113

name: A710
descrtn: THE FIRST LAW OF THERMODYNAMICS:AN APPLICATION OF HESS'S LAW
subject: FIRST YEAR DEGREE LEVEL EXPERIMENTAL LABORATORY
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE,BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 114

name: AG10 PARTS 1 AND 2
descrtn: KINETICS OF THE HYDROLYSIS OF SUGAR
subject: FIRST YEAR DEGREE LEVEL EXPERIMENTAL LABORATORY
comment: CALCHEM
lang: PART 1-STAF(BASED ON LEEDS AUTHOR LANGUAGE) PART 2-CALC
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 115

name: B101 PARTS 1 AND 2
descrtn: DISSOCIATION ENERGY OF I2 BY SPECTROSCOPIC METHODS
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE,BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 116

name: B102 2 PARTS
descrtn: HEAT CAPACITY OF SO2 FROM SPECTROSCOPIC MEASUREMENTS
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE,BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT.TEL 0532 31751 X 6089

Package ref no: 117

name: B102 2 PARTS
descrtn: HUCKEL MO CALCULATIONS
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: PART 1-STAF(BASED ON LEEDS AUTHOR LANGUAGE) PART 2-FORTRAN
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 118

name: B113 3 PARTS
descrip: INTRODUCTION TO MOLECULAR SPECTROSCOPY 1. BOND LENGTH OF CO
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: THE EXPERIMENTAL PLANNING SECTION OF THIS PROGRAM COMES IN
VERSIONS SUITABLE FOR USE WITH A GRUBB PARSONS SPECTROMASTER
A PERKINS ELMER 257 AND A UNICAM SP2000. IN ADDITION A
GENERAL VERSION NOT SPECIFYING ANY INSTRUMENT IS AVAILABLE
THE VERSION REQUIRED SHOULD BE SPECIFIED
lang: STAF AUTHOR LANGUAGE. BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P. AYS COUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 119

name: B218 3 PARTS
descrip: MAGNETOCHEMISTRY 1
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE. BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P. AYS COUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 120

name: B401 2 PARTS
descrip: LOW TEMPERATURE ADSORPTION ISOTHERM
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE. BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P. AYS COUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 121

name: B501 2 PARTS
descrip: DISSOCIATION CONSTANT OF ACETIC ACID
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: PART 1=STAF (BASED ON LEEDS AUTHOR LANGUAGE) PART 2=CALC
contact: PROFESSOR P. AYS COUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 122

name: B502 3 PARTS
descrip: ASSOCIATION CONSTANT OF FENCS2+
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: PART 1=STAF (BASED ON LEEDS AUTHOR LANGUAGE) PARTS 2 AND 3 ARE
IN CALC AND BASIC
contact: PROFESSOR P. AYS COUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 123

name: B584
descrip: EQUILIBRIA IN AQUEOUS SOLUTIONS
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 124
name: B511 2 PARTS
descrip: EFFECT OF IONIC STRENGTH ON SOLUBILITY
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE PART
2-BASIC
contact: PROFESSOR P. AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS LS2 9JT TEL 0532 31751 X 6889

Package ref no: 125
name: B683
descrip: FE2+/FE3+ REDOX SYSTEM
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 126
name: B618 2 PARTS
descrip: ION SELECTIVE ELECTRODES 1:THE F- ELECTRODE
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 127
name: B611 2 PARTS
descrip: ION SELECTIVE ELECTRODES 2:THE GLASS ELECTRODE
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 128
name: B881 2 PARTS
descrip: KINETICS OF THE DECOMPOSITION OF DI-UNDERGRADUATE BUTYL
PEROXIDE
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM

lang: PART1=STAF(BASED ON LEEDS AUTHOR LANGUAGE) PART2=FORTRAN OR
CALC
contact: PROFESSOR P. AYSICOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 129

name: 8984
descrip: KINETICS OF IODINATION OF ACETONE
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE, BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P. AYSICOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 130

name: 8985
descrip: KINETICS AND MECHANISM OF THE OXIDATION OF FORMIC ACID BY
BROMINE
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE, BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P. AYSICOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 131

name: 8986
descrip: TEMPERATURE JUMP
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE, BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P. AYSICOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 132

name: 8918 2 PARTS
descrip: EFFECTS OF IONIC STRENGTH ON RATE CONSTANTS
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: PART1=STAF(BASED ON LEEDS AUTHOR LANGUAGE) PART2=BASIC
contact: PROFESSOR P. AYSICOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 133

name: 8911 2 PARTS
descrip: RATE CONSTANTS FOR RADICAL COMBINATIONS
subject: 2ND YEAR DEGREE LEVEL CHEMISTRY, EXPERIMENTAL LAB
comment: CALCHEM
lang: PART1=STAF(BASED ON LEEDS AUTHOR LANGUAGE) PART2=BASIC OR
CALC
contact: PROFESSOR P. AYSICOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6889

Package ref no: 136

name: S167, S168, S167

description: INTERPRETATION OF SPECTRA. EACH PACKAGE CONTAINS A
SUBROUTINE OF A PROGRAM (S.C. TO COMPUTE THE CHEMICAL
SPECTRA INVOLVED IN A SEQUENCE OF REACTIONS), A LIST OF THE
INFORMATION WHICH THE STUDENT CAN OBTAIN FROM THE COMPUTER
AND INSTRUCTIONS ABOUT HOW TO REQUEST THE INFORMATION. THE
COMPUTER KEEPS RECORDS OF THE INFORMATION GIVEN TO THE
STUDENT, HELPS WITH INTERPRETATION OF REQUESTS, ENLIGHTENS THE
STUDENT TO GIVE THE SOLUTION WHEN HE HAS ENOUGH
INFORMATION, KEEPS A SCORE AND REQUESTS THE STUDENT TO GIVE
COMPARISON OF ANSWERS BASED ON PREVIOUS EVOLVED.

subject: PHYSICAL CHEMISTRY, ORGANIC CHEMISTRY

comments: CALCULATIONS

lang: SELF AUTHOR LANGUAGE, BASED ON LEADS AUTHOR LANGUAGE

contact: PROFESSOR P. AYSCOMBE, DEPT OF PHYSICAL CHEMISTRY, LEADS
UNIVERSITY, LEADS, LS2 9JT TEL 0532 31731 X 6888

Package ref no: 135

name: S161 2 PARTS

description: INTERPRETATION OF SPECTRA 1

subject: THIS SUITE IS BASED ON INTERPRETATION OF SPECTRA ORGANIC
LEVEL CHEMISTRY

comments: CALCULATIONS

lang: PART1=SELF, PART2=SELF (BASED ON LEADS AUTHOR LANGUAGE)

contact: PROFESSOR P. AYSCOMBE, DEPT OF PHYSICAL CHEMISTRY, LEADS
UNIVERSITY, LEADS, LS2 9JT TEL 0532 31731 X 6888

Package ref no: 136

name: S161 2 PARTS

description: INTERPRETATION OF SPECTRA 2

subject: THIS SUITE IS BASED ON INTERPRETATION OF SPECTRA ORGANIC
LEVEL CHEMISTRY

comments: CALCULATIONS

lang: PART1=SELF (BASED ON LEADS AUTHOR LANGUAGE) PART2=SELF OR
FORTRAN

contact: PROFESSOR P. AYSCOMBE, DEPT OF PHYSICAL CHEMISTRY, LEADS
UNIVERSITY, LEADS, LS2 9JT TEL 0532 31731 X 6888

Package ref no: 137

name: S168

description: INTERPRETATION OF SPECTRA 2

subject: THIS SUITE IS BASED ON INTERPRETATION OF SPECTRA ORGANIC
LEVEL CHEMISTRY

comments: CALCULATIONS

lang: SELF AUTHOR LANGUAGE, BASED ON LEADS AUTHOR LANGUAGE

contact: PROFESSOR P. AYSCOMBE, DEPT OF PHYSICAL CHEMISTRY, LEADS
UNIVERSITY, LEADS, LS2 9JT TEL 0532 31731 X 6888

Package ref no: 138

name: S161 2 PARTS

descrtn: INTERPRETATION OF MASS SPECTRA
subject: THIS SUITE IS BASED ON INTERPRETATION OF SPECTRA DEGREE
LEVEL CHEMISTRY
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 139

name: S901
descrtn: INTEGRATED SPECTROSCOPY 1
subject: THIS SUITE IS BASED ON INTERPRETATION OF SPECTRA DEGREE
LEVEL CHEMISTRY
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 140

name: Z101
descrtn: ANALYSIS BY GAS
subject: THIS SUITE IS BASED ON INTERPRETATION OF SPECTRA DEGREE
LEVEL CHEMISTRY
comment: CALCHEM
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 141

name: T113
descrtn: INTRODUCTION TO MOLECULAR SPECTROSCOPY
subject: THESE ARE SELF CONTAINED TUTORIAL PACKAGES DEGREE LEVEL
CHEMISTRY
comment: CALCHEM SIMULATION AND CALCULATION FACILITIES MAY BE USED
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 142

name: T512
descrtn: ACIDS BASES AND INDICATORS
subject: THESE ARE SELF CONTAINED TUTORIAL PACKAGES DEGREE LEVEL
CHEMISTRY
comment: CALCHEM SIMULATION AND CALCULATION FACILITIES MAY BE USED
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 143

name: T711
descrtn: BASIC THERMODYNAMICS

subject: THESE ARE SELF CONTAINED TUTORIAL PACKAGES DEGREE LEVEL
CHEMISTRY
comment: CALCHEM SIMULATION AND CALCULATION FACILITIES MAY BE USED
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 144
name: T210
descrtn: MAGNETOCHEMISTRY
subject: THESE ARE SELF CONTAINED TUTORIAL PACKAGES DEGREE LEVEL
CHEMISTRY
comment: CALCHEM SIMULATION AND CALCULATION FACILITIES
lang: STAF AUTHOR LANGUAGE.BASED ON LEEDS AUTHOR LANGUAGE
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 145
name: S902, Y201, Y211, X100
descrtn: THESE 4 PACKAGES ARE UNDER DEVELOPMENT.THEY ARE CONCERNED
WITH INTEGRATED SPECTROSCOPY 2, SYNTHESIS OF 2PHENYLPROPENE,
SYNTHESIS OF 4PHENYLBUTANOIC ACID AND X-RAY CRYSTALLOGRAPHY
RESPECTIVELY
subject: CHEMISTRY, DEGREE LEVEL
comment: CALCHEM
lang: NOT KNOWN AT PRESENT
contact: PROFESSOR P.AYSCOUGH, DEPT OF PHYSICAL CHEMISTRY, LEEDS
UNIVERSITY, LEEDS, LS2 9JT TEL 0532 31751 X 6089

Package ref no: 156
name: C1 THERMODYNAMICS
descrtn: CALCULATION AID FOR TWO REACTIONS.STUDENT INPUTS INITIAL
REACTION CONDITIONS.OUTPUT IS THE GIBBS FREE ENERGY,
ENTHALPY AND THE EQUILIBRIUM CONSTANT
subject: CHEMISTRY:UNDERGRADUATE
comment: TELETYPE
lang: BASIC
contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 157
name: C2 MONOBASIC/DIBASIC ACIDS
descrtn: INPUT=DISSOCIATION CONSTANTS AND SOLUTION CONCENTRATION
OUTPUT=1ST AND 2ND APPROX. OF THE HYDROGEN ION CONC.
subject: CHEMISTRY:UNDERGRADUATE
comment: TELETYPE
lang: BASIC
contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 158

name: C3 PARTICLE IN A POTENTIAL WELL
descrtn: INPUT=PARTICLE MASS, WELL WIDTH AND HEIGHT
OUTPUT=GRAPHIC=ENERGY LEVELS IN SUCH A SQUARE WELL AND ALSO
SQUARE WELL OF INFINITE HEIGHT
subject: CHEMISTRY:UNDERGRADUATE
lang: BASIC
contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 159

name: C4 BOLTZMAN DISTRUBUTION
descrtn: LABORATORY EXERCISE TO SIMULATE ENERGY TRANSFER
subject: CHEMISTRY:UNDERGRADUATE
comment: TELETYPE
lang: BASIC AND FORTRAN
contact: DR.T.MOON, UNIVERSITY COLLEGE.GOWER ST, LONDON WC1E 6BT TEL
01 387 7050

Package ref no: 160

name: C5 BOLTZMAN DISTRIBUTIONS OF ENERGIES AND SPEEDS OF A GAS
descrtn: TWO PARTS.ONE DISPLAYS THE SPEED DIST. AND REQUIRES THE
STUDENT TO INPUT THE MOLECULAR WEIGHT AND TEMP. OF THE GAS.
THE OTHER DISPLAYS THE DISTRIBUTION OF ROTATIONAL ENERGY OF
LINEAR MOLECULES, ONCE THE ROTATIONAL CONSTANT AND
TEMPERATURE ARE SPECIFIED.
subject: CHEMISTRY:UNDERGRADUATE
comment: TELETYPE
lang: BASIC
contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 161

name: C6 KVIST
descrtn: LECTURE DEMONSTRATION.USED AS A DATA FITTING PROGRAM TO
DEMONSTRATE THE RELATIONSHIP BETWEEN EQUILIBRIUM CONSTANT
AND TEMPERATURE.
subject: CHEMISTRY:UNDERGRADUATE
lang: BASIC
contact: R.CHAPMAN, CHELSEA COLLEGE, MANRESA RD, LONDON SW3 6LX TEL
01 352 6421

Package ref no: 162

name: C7 PTSYM
descrtn: THE STUDENT CAN SELECT A SYMMETRY OPERATION AND SEE A 3-D
REPRESENTATION OF THIS ON THE SCREEN.IT IS THEN POSSIBLE TO
BUILD UP COMPLEX GROUPS FROM THE CUMULATIVE OPERATIONS.A
SECOND PACKAGE PERMITS STUDENTS TO SELECT ANY POINT ON THE
SURFACE OF A SPHERE AND INDICATES HOW THE CORRESPONDING 2-D
STEREOGRAM IS OBTAINED.
subject: CHEMISTRY:UNDERGRADUATE
lang: BASIC AND FORTRAN

contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 163

name: C10 GAUSS

descrtn: BASED ON BREAKDOWN AND BUILD UP OF GAUSSIAN CURVES.IN 3
PARTS.PART1=ADDITION, PART2=DEDUCTION OF PARAMETERS, PART3
USES STUDENT EXPERIMENTAL DATA.

subject: CHEMISTRY:UNDERGRADUATE

lang: BASIC

contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 164

name: C11 FREE ENERGY

descrtn: LECTURE DEMONSTRATION:PLOTS CHANGE IN GIBBS FREE ENERGY
VERSUS REACTANT CONCENTRATION FOR A GIVEN REACTION AT A
FIXED TEMPERATURE.

subject: CHEMISTRY:UNDERGRADUATE

lang: BASIC

contact: DR.T.MOON, UNIVERSITY COLLEGE.GOWER ST, LONDON WC1E 6BT TEL
01 387 7050

Package ref no: 165

name: C12 HARMONIC

descrtn: 3PART PACKAGE:1) DISPLAYS THE CLASSICAL POTENTIAL ENERGY
CURVE, QUANTISED ENERGY LEVELS AND THEIR ASSOCIATED EIGEN
FUNCTIONS.2) COMPARES THE SHAPE OF THE CLASSICAL POTENTIAL
ENERGY CURVE WITH THE MORSE CURVE.3) DISPLAYS THE ANHARMONIC
OSCILLATOR CURVE AND ENERGY LEVELS UP TO THE DISSOCIATION
ENERGY

subject: CHEMISTRY:UNDERGRADUATE

lang: BASIC

contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 166

name: C13 ELECTROLYTIC CONDUCTANCE

descrtn: THE STUDENT CHOOSES A SOLUTE AND A SOLVENT AND THEN, BY
VARYING THE CONDUCTANCE AT INFINITE DILUTION AND THE ION
SIZE PARAMETER, ATTEMPTS TO FIT THEORETICAL EXPRESSIONS TO
THE EXPERIMENTAL DATA

subject: CHEMISTRY UNDERGRADUATE

lang: BASIC

contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD,
SURREY.TEL 0483 71281 X 322

Package ref no: 167

name: C15.1 ATOM

descrtn: THE STUDENT SPECIFYS THE ATOMIC ORBITAL, THE EFFECTIVE
NUCLEAR CHARGE AND THE SCALE.THE PROGRAM GENERATES SHADED

CONTOUR DISPLAYS OF HYDROGEN-LIKE ATOMIC ORBITALS. IN ADDITION ON REQUEST, THE FOLLOWING FUNCTIONS ARE DISPLAYED: THE RADIAL PART OF THE WAVE FUNCTION, THE RADIAL DISTRIBUTION FUNCTION, AND THE TOTAL WAVE FUNCTION ALONG ANY CHOSEN DIRECTION FROM THE NUCLEUS.

subject: CHEMISTRY:UNDERGRADUATE
lang: BASIC AND FORTRAN
contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD, SURREY.TEL 0483 71281 X 322

Package ref no: 168

name: CI5.2 MPlot

descrtn: THE STUDENT SPECIFIES THE TYPE OF MOLECULAR ORBITAL, THE NUCLEAR CHARGE, THE NUCLEAR SEPARATION AND THE SCALE. OUTPUT= SHADED MOLECULAR ORBITAL PLOTS FOR HOMONUCLEAR DIATOMIC MOLECULES FOR THE APPROPRIATE COMBINATIONS OF 1S, 2S AND 2P ATOMIC ORBITALS

subject: CHEMISTRY:UNDERGRADUATE

comment: TELETYPE

lang: BASIC

contact: D.LAURILLARD, I.E.T., UNIVERSITY OF SURREY, GUILDFORD, SURREY. TEL 0483 71281 X 322.

Package ref no: 169

name: CI5.2 MLOB

descrtn: AS FOR CI5.2 MPlot AT SURREY BUT GRAPHICAL, OTHER FACILITIES INCLUDE HETERO-NUCLEAR DIATOMICS. ALSO 1S, 2S, 2PX, 2PY, 3DXY ORBITALS CAN BE USED TO CONSTRUCT HYBRID OF MOLECULAR ORBITALS, PLUS LINE PLOTS OF THE CONTRIBUTORY OR TOTAL WAVE FUNCTION.

subject: CHEMISTRY:UNDERGRADUATE

lang: BASIC

contact: R.CHAPMAN, CHELSEA COLLEGE, MANRESA RD, LONDON SW3 6LX TEL 01 352 6421

Package ref no: 189

NAME:

descrtn: LIBRARY OF PROGRAMS IN BIOLOGY, CHEMISTRY, CIVIL ENGINEERING HOTEL AND CATERING MANAGEMENT AND TOURISM, LINGUISTICS AND REGIONAL STUDIES, MATHEMATICS, PHYSICS, PSYCHOLOGY, SOCIOLOGY AND STATISTICS

subject: VARIOUS.AS ABOVE

comment: RUN BY COMPUTER CENTER AND CONCERNED WITH PROVIDING A UNIVERSITY WIDE CAL SERVICE, BUILDING ON TWO EXISTING NDPCAL FUNDED PROJECTS, COMPUTATIONAL PHYSICS TEACHING LABORATORY AND COMPUTERS IN THE UNDERGRADUATE SCIENCE CURRICULUM

lang: BASIC AND FORTRAN

contact: T.F.GOODWIN, HEAD OF COMPUTING UNIT, UNIVERSITY OF SURREY, GUILDFORD, SURREY, GU2 5XH TEL 0483 71281

Package ref no: 208

name: ABTCPP
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: TITRATION GRAPH OF PH V VOLUME
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 209

name: ACIDBASE
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: COMPUTATION OF THE THEORETICAL PH TITRATION CURVE FOR THE
ADDITION OF A MONOACIDIC BASE TO A MONOBASIC ACID
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 210

name: ASYRATOR
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES PRINCIPLE MOMENTS OF INERTIA ETC FOR ASYMETRIC
ROTOR MOLECULES
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 211

name: BEE2
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES P1-ELECTRON DENSITIES AND BOND ORDERS OF
MOLECULES BY THE HUCKEL METHOD
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 212

name: BEE5
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES KINETIC PARAMETERS OF SOLID STATE DECOMPOSITION
REACTIONS FROM DIFFERENTIAL SCANNING CALORIMETRY DATA
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902

27371

Package ref no: 213

name: BEE7
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES ABSOLUTE(TRUE) MELTING POINTS FROM DIFFERENTIAL
SCANNING CALORIMETER DATA
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 214

name: BEECHU
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES ENERGY OF IONIC SOLID AS FUNCTION OF INTERIONIC
DATA
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 215

name: BEMONTE
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: MONTE CARLO SIMULATION OF A REACTION
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 216

name: BOLTM
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES OCCUPANCY OF THE VIBRATIONAL LEVEL OF A DIATOMIC
GAS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 217

name: BXTL
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: EVALUATES CRYSTAL-FIELD SPLITTING PARAMETER (10 DQ) AND
RACAH PARAMETER (B)
subject: CHEMISTRY, UNDERGRADUATE LEVEL

lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 218

name: C317
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES DISTANCE OF CLOSEST APPROACH OF IONS AND
THERMODYNAMIC ION PAIR ASSOCIATION CONSTANT FOR SYMMETRICAL
ELECTROLYTES
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: ALGOL
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 219

name: CHER
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES THE VISCOSITY AVERAGE MOLECULAR WEIGHT OF A
THERMOPLASTIC
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 220

name: CONT
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: MODIFICATION OF NEWPLOT FOR USE ON TELETYPE
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 221

name: CRVY
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES END POINTS IN POTENTIOMETRIC OR PH TITRATIONS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 222

name: ELECTRODE
author: CENTRAL PROGRAM EXCHANGE(CPE)

descrtn: CALCULATES STANDARD ELECTRODE POTENTIAL
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 223

name: ELSPEC
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: ASSISTS IN CALCULATION OF MOLECULAR PARAMETERS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 224

name: FORCON
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: COMPUTES VIBRATIONAL FORCE CONSTANTS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: ALGOL
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 225

name: FORDER
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: INVESTIGATES CHANGES IN CONCENTRATION OF A REACTANT UNDER A
FIRST ORDER REACTION
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 226

name: FORTRAT
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: DEALS WITH THE ROTATIONAL FINE STRUCTURE OF ELECTRONIC BANDS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 227

name: H202K

author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES RATE CONSTANTS AND ACTIVATION ENERGY FOR THE 1ST
ORDER IRON(3) CATALYSED DECOMPOSITION OF HYDROGEN PEROXIDE
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 228

name: H2PLUS
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: EVALUATES THE ENERGY OF THE BONDING AND ANTI-BONDING
ORBITALS OF H_2^+ FOR SPECIFIED VALUES OF THE BOND LENGTH AND
OF THE IS ORBITAL EXPONENT
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 229

name: HATO
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: MODIFICATION OF NEWPLOT PLOTS ELECTRON DENSITY MAP OF
HYDROGEN MOLECULE ION
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 230

name: HM01
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES THE SHAPE OF THE CLUSTER OF PEAKS PRODUCED IN A
MASS SPECTROMETER
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 231

name: INTEGRAL
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: EVALUATES AUXILIARY INTEGRALS A AND B WHICH ARISE IN
CALCULATIONS ON DIATOMIC MOLECULES
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE

POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0982 27371

Package ref no: 232

name: IR2
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: ASSISTS IN LEARNING OF THE TECHNIQUE OF INFRA-RED SPECTRAL INTERPRETATION BY A QUESTION AND ANSWER METHOD
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0982 27371

Package ref no: 233

name: KMT
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES RATE PARAMETERS FOR A PERSULPHATE-IODIDE REACTION
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0982 27371

Package ref no: 234

name: LAOC
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: TWO PARTS:A-CALCULATES PEAK HEIGHTS AND POSITIONS IN NMR SPECTRUM GIVEN COUPLING CONSTANTS AND CHEMICAL SHIFTS
B-OBTAINS CONSTANTS AND SHIFTS FROM AN INPUT SPECTRUM
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0982 27371

Package ref no: 235

name: LIND
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: IDENTIFIES COMPOUND BY COMPARISON OF ITS MOST PROMINENT IR AND NMR PEAKS WITH THOSE STORED BY THE PROGRAM LOAD. MOST PROBABLE ASSIGNMENT IS MADE, TOGETHER WITH THE LESS LIKELY ONES, BASED ON A POINT SCORING SYSTEM
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0982 27371

Package ref no: 236

name: LOAD

author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: DATA STORAGE OF NAME OF COMPOUND, IR PEAKS AND NMR PEAKS 5
subject: MOST PROMINENT PEAKS ARE STORED USED WITH PROGRAM LIND
lang: CHEMISTRY, UNDERGRADUATE LEVEL
contact: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LV TEL 0902
27371

Package ref no: 237

name: LUCK
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: CALCULATES ELECTRIC DIPOLE MOMENTS FROM MEASUREMENTS IN
subject: SOLUTION
lang: CHEMISTRY, UNDERGRADUATE LEVEL
contact: ALGOL
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LV TEL 0902
27371

Package ref no: 238

name: MADCON
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: CALCULATES MADELUNG CONSTANTS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: ALGOL
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LV TEL 0902
27371

Package ref no: 239

name: MINISQUAD
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: COMPUTES FORMATION CONSTANT FROM POTENTIOMETRIC DATA
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LV TEL 0902
27371

Package ref no: 240

name: MULT
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: CALCULATES CONCENTRATIONS OF COMPONENTS IN A MIXTURE
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LV TEL 0902
27371

Package ref no: 241

name: NEWPLOT
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: PRODUCES LINE PRINTER REPRESENTATIONS OF ATOMIC ORBITALS
EITHER NUMERICALLY OR SYMBOLICALLY, ANY ORBITAL, ANY CHARGE
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BESCH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 242

name: ORGCRN, ORCRUN
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: PAIR OF PROGRAMS DEMONSTRATING QUALITATIVE TECHNIQUES IN
ORGANIC ANALYSIS AT AN ELEMENTARY LEVEL
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BESCH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 243

name: PRC1
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: USED IN CONJUNCTION WITH EXPERIMENTAL LABORATORY ORGANIC
REACTION MECHANISMS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BESCH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 244

name: FEES
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: SIMULATES APPEARANCE OF PARENT PEAK REGION OF THE MASS
SPECTRUM OF A COMPOUND
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BESCH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 245

name: FENT
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrip: TO OBTAIN SIMULATED TITRATION CURVES FOR COMPARISON WITH
CURVES OBTAINED IN PRACTICAL WORK, OR FOR LECTURE MATERIAL
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BESCH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE

POLYTECHNIC, WILFRIDA ST. WOLVERHAMPTON WV1 1LB TEL 0902 27371

Package ref no: 246

name: PLATE

author: CENTRAL PROGRAM EXCHANGE (CPE)

description: IMPUT-OUTPUTS POINTS + DATA OF FUNCTION-OUTPUTS OF THE
SOURCES OF LISTS AND COLS V AND COMPOSITION AT A SOURCE
OF THEORETICAL

subject: CHEMISTRY, UNDERGRADUATE LEVEL

lang: FORTRAN 4

contact: DR. G. BERRY, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WILFRIDA ST. WOLVERHAMPTON WV1 1LB TEL 0902 27371

Package ref no: 247

name: RUT

author: CENTRAL PROGRAM EXCHANGE (CPE)

description: CALCULATION OF -LOG CONC. AT VARIOUS POINTS OF A TITRATION
OF AN ACID (OR TO TRIASIS) WITH A MONO-ACID BASE

subject: CHEMISTRY, UNDERGRADUATE LEVEL

lang: FORTRAN 4

contact: DR. G. BERRY, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WILFRIDA ST. WOLVERHAMPTON WV1 1LB TEL 0902 27371

Package ref no: 248

name: PLATE

author: CENTRAL PROGRAM EXCHANGE (CPE)

description: ASSISTS IN TEACHING OF THEORETICAL PLATE CONCEPT AS APPLIED
TO THE DISTILLATION OF A 2-COMPONENT IDEAL SYSTEM

subject: CHEMISTRY, UNDERGRADUATE LEVEL

lang: BASIC

contact: DR. G. BERRY, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WILFRIDA ST. WOLVERHAMPTON WV1 1LB TEL 0902 27371

Package ref no: 249

name: POLI

author: CENTRAL PROGRAM EXCHANGE (CPE)

description: SUBROUTINE TO ANALYSE POLYMERIZATION DATA

subject: CHEMISTRY, UNDERGRADUATE LEVEL

lang: FORTRAN

contact: DR. G. BERRY, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WILFRIDA ST. WOLVERHAMPTON WV1 1LB TEL 0902 27371

Package ref no: 250

name: POT

author: CENTRAL PROGRAM EXCHANGE (CPE)

description: DETERMINES END POINT OF A POTENTIAL METRIC TITRATION DATA

CSDA PROJECT

IMPERIAL COLLEGE

subject: TAKEN FROM LABORATORY EXPERIMENT
lang: CHEMISTRY, UNDERGRADUATE LEVEL
contact: BASIC
DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 251
name: QUALO
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: SIMULATION OF QUALITATIVE ORGANIC ANALYSIS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC AND FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 252
name: RCPI
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES RATE CONSTANT FOR MUTAROTATION
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 253
name: SOLU
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES ENTHALPY OF SOLUTION
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 254
name: SPAN
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: ACCEPTS A DIGITISED NMR SPECTRUM AND 1) REDRAWS TO ANY SIZE
2) IDENTIFYS PEAKS AND CALCULATES PEAK AREAS 3) EDITS THE
SPEC
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 255
name: SPEK

author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: ACCEPTS DIGITAL RECORD(PAPER TAPE) FROM ATOMIC ABSORPTION
MEASUREMENT AND CORRECTS FOR NOISE AND BASELINE SLOPE
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 256

name: SYNCRE, SYN RUN
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: PAIR OF PROGRAMS DEMONSTRATES USES OF REAGENTS FOR SINGLE-
STEP ORGANIC SYNTHESIS
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 257

name: VAPO
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: OBTAINS ENTHALPIES OF VAPOURISATION OF SOLIDS/LIQUIDS BY
CLAUSIUS/CLAPEYROW EQUATION, USES DATA FROM ISOTENISCOPE.
subject: CHEMISTRY, UNDERGRADUATE LEVEL
lang: FORTRAN 4
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 279

name: ARLP
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: ANALYTIC REFINEMENT OF LATTICE PARAMETERS
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: ALGOL 60
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 280

name: BONDLA
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATION OF INTER ATOMIC DISTANCES
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 281

name: CHAIN
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: RADIOACTIVE DECAY CHAIN
subject: NUCLEAR CHEMISTRY AND X-RAY
comment: SEE ALSO UNIVERSITY OF SURREY MATERIAL PHYSICS DEPT.
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 282

name: COUNTERS
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: STUDY OF THE MERITS OF DIFFERENT COUNTING SYSTEMS FOR
VARIOUS ISOTOPES
subject: NUCLEAR CHEMISTRY AND X-RAY
comment: SEE COUNTERS.PH, SURREY PHYSICS
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 283

name: DVAL
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: CALCULATES INTER-PLANAR SPACINGS
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 284

name: ESP19
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: BASED ON SEMI-EMPIRICAL BINDING ENERGY AND NEUTRON
ADSORPTION
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 285

name: FOURIER
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: COMPUTES AND INTERPRETS ELECTRON DENSITY PROJECTION
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: ALGOL
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE

POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 286

name: GHMC
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: GENERATES THE POSITION(S) OF HYDROGEN ATOM(S) ON SP2,
3CARBON
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 287

name: HAL1
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: CALCULATES HALFLIFE FROM ACTIVITY VALUES
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 288

name: HX60
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: REFINES APPROXIMATE UNIT CELL DIMENSIONS FROM X-RAY POWDER
DIFFRACTION DATA
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 289

name: HX88
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: PRODUCES BALL AND STICK PERSPECTIVE DRAWINGS OF A MOLECULE
FROM ANY SPECIFIED VIEWPOINT
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 290

name: LMPF
author: CENTRAL PROGRAM EXCHANGE(CPE)
descrtn: LOCATES PEAK POSITION FROM VALUES OF FUNCTION(E.G. ELECTRON
DENSITY) AT GRID POINTS SURROUNDING IT

subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 291

name: PBAC
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: CALCULATES BOND DISTANCES AND ANGLES FROM GIVEN AUTOMATIC
CO-ORDINATES IN X-RAY PAPERS
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: FORTRAN
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 292

name: ROXRAY
author: CENTRAL PROGRAM EXCHANGE (CPE)
descrtn: SIMULATION OF X-RAY PRODUCTION
subject: NUCLEAR CHEMISTRY AND X-RAY
lang: BASIC
contact: DR.G.BEECH, DEPT OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST.WOLVERHAMPTON WV1 1LY TEL 0902
27371

Package ref no: 330

name: SELF CORRECTING CHEMISTRY TEST
descrtn: 10 QUESTIONS ON IDEAL GAS LAW, 1 MASS PROBLEM AND FINALLY 10
MORE GAS LAW PROBLEMS
subject: CHEMISTRY
docs: SOME + SUPPORT
lang: BASIC
contact: K.C.AINSOE, COMPUTER CENTRE, BLACKBURN COLLEGE OF
TECHNOLOGY AND DESIGN, FIELDEN ST., BLACKBURN BB2 1LH TEL
BLACKBURN 64321

Package ref no: 331

name: HABER
descrtn: ENABLES STUDENTS TO DISCOVER FOR THEMSELVES HOW VARIOUS
CONDITIONS AFFECT AMMONIA PRODUCTION
subject: CHEMISTRY SECONDARY
docs: SOME+SUPPORT+TEST DATA
comment: SOFTWARE FREE TO PURCHASERS OF PACKS (6 STUDENT NOTES , 1
TEACHERS GUIDE) . \$5.50 PER PACK
lang: BASIC
contact: EDWARD ARNOLD (PUBLISHERS) LTD., CHELSEA SCIENCE SIMULATION
PROJECT, CHELSEA CENTRE FOR SCIENCE EDUCATION UNIVERSITY OF
LONDON, BRIDGES PLACE, LONDON SW6 4HR

Package ref no: 332

name: RKINET
descrtn: TWO BASIC OBJECTIVES 1) EXTEND A STUDENT'S LAB. EXPERIENCE AND UNDERSTANDING OF REACTION KINETICS BY ENABLING CARRYING OUT OF A WIDER RANGE OF INVESTIGATIONS THAN NORMALLY PRACTICABLE AND TO ASSIST UNDERSTANDING OF THE RELATIONSHIP BETWEEN MATHEMATICAL MODEL AND REALITY.
subject: CHEMISTRY SECONDARY
docs: SOME+SUPPORT+TEST DATA
comment: SOFTWARE FREE TO PURCHASERS OF PACKS (6 STUDENT NOTES , 1 TEACHERS GUIDE) . \$5.50 PER PACK
lang: BASIC
contact: EDWARD ARNOLD(PUBLISHERS) LTD., CHELSEA SCIENCE SIMULATION PROJECT, CHELSEA CENTRE FOR SCIENCE EDUCATION UNIVERSITY OF LONDON, BRIDGES PLACE, LONDON SW6 4HR

Package ref no: 333

name: LAT2
descrtn: SHOWS HOW THE SHAPE OF THE POTENTIAL ENERGY CURVE CHANGES AS THE INTERIONIC DISTANCE IS VARIED
subject: CHEMISTRY UNDERGRADUATE
docs: NONE:FORTAN SOURCE DECK ONLY
lang: FORTRAN
contact: J.D.LEE, UNIVERSITY OF LOUGHBOROUGH, LEICESTER, TEL 0503 63171

Package ref no: 341

name: QUALITATIVE ORGANIC ANALYSIS
descrtn: ANALYSES, THROUGH QUESTION AND ANSWER, ORGANIC COMPOUNDS
subject: CHEMISTRY UNDERGRADUATE
docs: SOME+SUPPORT+TEST DATA
lang: FORTRAN
contact: K.C.AINSOE, COMPUTER CENTRE, BLACKBURN COLLEGE OF TECHNOLOGY AND DESIGN, FIELDEN ST., BLACKBURN BB2 1LH TEL BLACKBURN 64321

Package ref no: 345

name: MSS2
descrtn: ALLOWS EVALUATION OF EFFICIENCY OF AN ANTIBIOTIC OR DISINFECTANT AGAINST VARIOUS ORGANISMS
subject: BIOCHEMISTRY UNDERGRADUATE
docs: SOME
lang: FORTRAN 4
contact: J.D.LEE, UNIVERSITY OF LOUGHBOROUGH, LEICESTER, TEL 0503 63171

Package ref no: 364

name: COLU
author: DR.G.BEECH
descrtn: ENTHALPY CALCULATIONS
subject: CHEMISTRY UNDERGRADUATE

docs: SOME+TEST DATA+SUPPORT
lang: FORTRAN
contact: DR.G.BEECH, DEPT.OF COMPUTING AND MATHEMATICAL SCIENCES, THE
POLYTECHNIC, WULFRUNA ST., WOLVERHAMPTON, WV1 1LY TEL 0902
27371